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HIGH-TEMPERATURE MCNP CROSS SECTIONS

by

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Los Alamos National Laboratory
Radiation Transport Group Informal Report

X-6-IR-87-505

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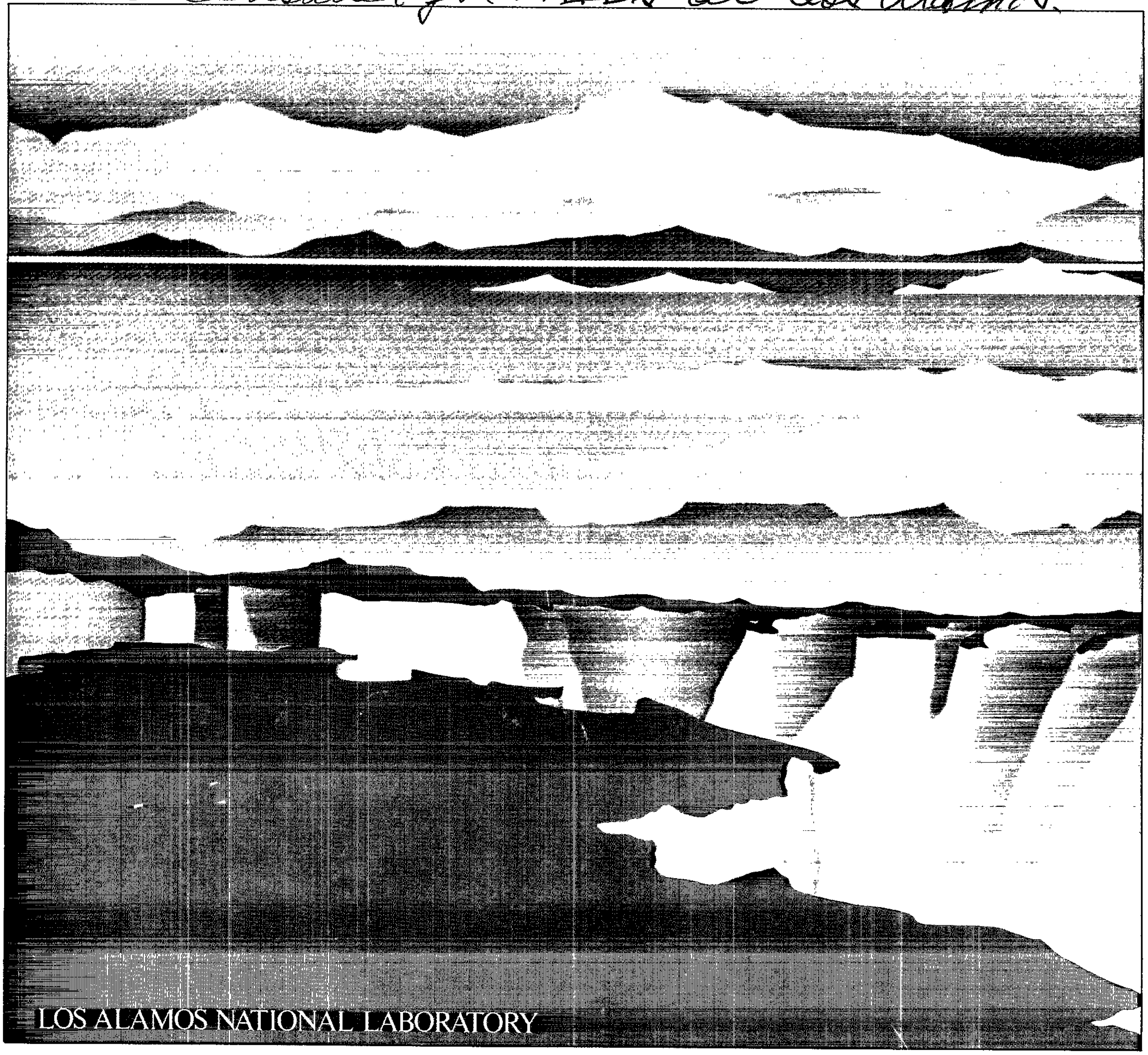
MCNP Version 3B Newsletter X-6:JFB-88-292
to be consulted for ZAIDs at Los Alamos.



Work performed in support of EPRI Agreement RP 2420-55

ABSTRACT

Neutron cross sections for several isotopes from ENDF/B-V have been Doppler broadened to reactor temperatures and processed into a format appropriate for the MCNP Monte Carlo code. Cross sections for ^{1}H, ^{10}B, ^{16}O, Zr, ^{135}Xe, ^{235}U, and ^{238}U have been made available at 600°K, and cross sections for ^{16}O, ^{135}Xe, ^{235}U, and ^{238}U have been made available at 900°K. The data libraries have been thoroughly tested, found satisfactory, and transmitted to S. Levy Inc. in accordance with the Electric Power Research Institute contract that funded this work.

On Nov 16, 1989 RCL gave us the following files for the cross sections and directories for the 12 reactor-temperature tables advertised in the MCNP Version 3B Newsletter (X-6:JFB-88-292)

/X6XS/CTSS/1/EPRIDIR1
/X6XS/CTSS/1/EPRIXS1

/X6XS/CTSS/2/EPRIDIR2
/X6XS/CTSS/2/EPRIXS2

I. INTRODUCTION

In May 1987, the Los Alamos National Laboratory (LANL) entered into an agreement[1] with the Electric Power Research Institute (EPRI) to provide high-temperature neutron cross-section libraries for the MCNP[2] Monte Carlo code. (EPRI Agreement RP2420-55; LANL Proposal X-DO-871). The original contract provided for $12,560. Because of additional calculations performed at Los Alamos, the contract has since been amended[3] to include an additional $5000.

The final cross-section libraries and associated files were transmitted to L. Eisenhart of S. Levy Inc. in July 1987. Many successful MCNP calculations have since been performed with the high-temperature libraries. This report serves as complete documentation of the preparation, checking, and testing of the new libraries.

The organization of this report is as follows. Section II will describe the data processing. Section III will summarize the differential and integral testing of the libraries. Section IV indicates the availability of the data and how one uses the data in MCNP. Section V contains results of reactor calculations performed at Los Alamos. Section VI is a summary of the work.

II. PROCESSING

A. ENDF/B-V EVALUATIONS

All cross-section evaluations are from ENDF/B-V Revision 0.[4] The MAT identifiers and the ENDF/B-V tapes from which the evaluations were taken are explicitly listed in Table I.

TABLE I

SOURCE OF ENDF/B-V CROSS-SECTION EVALUATIONS

Isotope	MAT	TAPE
H-1	1301	511
B-10	1305	511
O-16	1276	505
Zr	1340	508
Xe-135	1294	509
U-235	1395	511
U-238	1398	516

B. RECONR

The bulk of the data processing has been carried out with the NJOY[5] system. The next several sections describe the actual processing.

The RECONR module of NJOY reconstructs pointwise cross sections from resonance parameters. The module also linearizes any cross sections originally specified with non-linear interpolation. A unified energy grid is constructed that is sufficiently dense that linear interpolation preserves all cross sections to within a specified tolerance. A sample of our RECONR input file is contained in Fig. 1. All resonance cross sections were reconstructed at 0°K. ERRMAX, the fractional reconstruction tolerance used when the RECONR resonance-integral criterion is satisfied, was set to 0.001 (0.1%) for all isotopes except ^{238}U. Because of the large number of resolved resonances, ERRMAX for ^{238}U was raised to 0.02 (2%). This still resulted in over 80,000 points in the ^{238}U energy grid produced by RECONR. For all isotopes, ERR, the fractional reconstruction tolerance used when the RECONR resonance-integral error criterion is not satisfied, was set to 0.001 (0.1%). For a full discussion of the ERR and ERRMAX variables, see Ref. 6.

C. BROADR

The BROADR module performs Doppler broadening and thinning of the pointwise cross sections. The "kernel-broadening" technique is used. We have broadened the cross sections for each isotope to the temperatures listed in Table II. Notice that we have included room temperature (300°K) for all isotopes. This was done despite the fact that room-temperature

TABLE II

PROCESSED TEMPERATURES FOR EACH ISOTOPE

Isotope	Temperatures (°K)
H-1	300,600
B-10	300,600
O-16	300,600,900
Zr	300,600
Xe-135	300,600,900
U-235	300,600,900
U-238	300,600,900

ENDF/B-V cross-section sets already exist for MCNP for all isotopes of interest except ^{135}Xe. The room-temperature cross sections were regenerated primarily for reasons of consistency. When looking for small differences in calculated results, it may be important that the same processing code, same human processor, and same input tolerances and parameters have been used for all data sets. None of this would have been the case when comparing newly-generated high-temperature cross sections with ~1979-generated room-temperature cross sections. Hence, the additional processing of all seven isotopes at 300°K.

A sample of our BROADR input is contained in Fig. 1. The fractional tolerance for thinning, ERRTHN, in all cases was 0.001 (0.1%). Cross sections were broadened for elastic scattering, fission, radiative capture, and other absorption reactions (e.g., (n,p), (n,α), and (n,t2α) for ^{10}B).

D. HEATR

The HEATR module is used to calculate average pointwise values of energy deposition. Local energy deposition (heat) from neutron reactions is in the form of emitted charged particles or the kinetic energy of the recoil nucleus. HEATR generates energy-deposition values for all available temperatures. A sample of the HEATR portion of the NJOY input is shown in Fig. 1.

The HEATR module was the last module executed in the preparation of a PENDF (pointwise ENDF) tape for each isotope. The remaining modules of NJOY (GROUPR and ACER; described below) are executed to prepare data in a format suitable for MCNP.

E. GROUPR

When preparing cross-section libraries for MCNP, the purpose of the GROUPR module of NJOY is to produce neutron-induced photon-production matrices. These matrices are then used as the basis for calculating 20 equally-likely photon energies for each of 30 neutron groups. Although this method of producing photons from neutrons in MCNP is obsolete, the GROUPR module must still be executed for ACER to function properly. A sample GROUPR input may be found in Fig. 2.

F. ACER

ACER is the final NJOY module executed in the current sequence. ACER prepares the data library for MCNP. Energy-dependent cross sections, angular distributions, and energy distributions are processed as necessary and written out in a format appropriate for MCNP. Photon-production data, if available, are handled in a similar fashion. Pointwise cross sections are thinned so that linear-linear interpolation between adjacent energies (as assumed by MCNP) is sufficient to reproduce the original cross section to a user-specified tolerance, ERR. We have set ERR=0.001 (0.1%) for all processing. A sample of the ACER portion of the NJOY input is shown in Fig. 2.

G. ADDGAM

Execution of the ACER module completes the NJOY processing. ADDGAM is the first of several codes to be described that are used for additional processing and checking of the data tables. ADDGAM incorporates expanded photon-production data[7] into the cross-section tables by merging information from ENDF/B tapes with the ACER output files.

It may be noted that the capabilities of ADDGAM have been incorporated into NJOY, and, as such, ADDGAM is no longer explicitly required. However, there are slight differences between expanded photon-production data as determined by NJOY and expanded photon-production data as determined by ADDGAM. We have chosen the ADDGAM output in all cases.

H. ADDXS

The ADDXS code is used to add particle-production (p,d,t,^{3}He,α) cross sections to an existing data table. These particle-production cross sections are then available as response functions to be used with the FM feature of MCNP. The particle-production cross sections added, and the original reaction MTs from which they were formed, are listed in Table III. No particle-production cross sections are available for ^{135}Xe, ^{235}U, or ^{238}U.

TABLE III

PARTICLE-PRODUCTION CROSS SECTIONS

Isotope	Particle-Production MT	Particle	Original Reaction MTs
H-1	204	d	102
B-10	203	p	65,78,103
	204	d	62,64,68,70,71,73,74, 76,77,(79-81),83,84, 104
	205	t	113
	207	α	55,56,(58-61),63,66, 67,69,72,75,82,85, 107,2*[62,64,68,70, 71,73,74,76,77,(79-81),83,84,113]
O-16	203	p	67,71,74,76,79,81,84, 86,88,103
	204	d	104
	207	α	(56-58),(61-66),(68-70),72,73,75,77,78, 80,82,83,85,87,89, 107
Zr	203	p	103
	207	α	107

I. ADDCOL2

Two classes of neutron transport tables have traditionally been provided for MCNP: full continuous-energy and discrete reaction. The discrete-reaction tables have cross sections represented in a histogram form over 262 energy groups, and are designed for energy regimes where self-shielding is unimportant. Discrete cross sections are not to be confused with multigroup cross sections. The methods and data used to sample scattered energies and directions are identical to the methods and data used in the fully continuous sets.

The code ADDCOL2 has been used to generate discrete-reaction cross-section sets for each isotope and temperature listed in Table II. A comparison of discrete and continuous cross sections for ^{235}U fission from 0-100 eV is shown in Fig. 3.

J. LIBRARIES AND DIRECTORIES

At his point, all that remained to prepare the data for use in MCNP was to combine the individual data tables onto libraries and to produce the required cross-section directory files. That was easily accomplished. At Los Alamos, libraries in Type-3 (ACE) and Type-1 (BCD) format were prepared. (See Appendix F of Ref. 2 for a description of Type-1 and Type-3 formats). Associated directories were prepared as well. The Type-1 cross section directory is shown in Fig. 4.

III. DATA VERIFICATION AND TESTING

A. INTEGRAL DATA TESTING - MARK AND MRKACR

The MRKACR code[8] calculates group-averaged cross sections from an MCNP library with user-supplied group boundaries and weight spectrum. We have used MRKACR to calculate 30-group cross sections for each of the continuous-energy tables prepared during this work. An additional code was written to compare two sets of MRKACR output. All comparisons indicate reasonable results; i.e., any differences between two data sets for the same isotope occur at low energy and are explained by the different processing temperatures. As an example, the 30-group total cross sections of ^{10}B at 300° and 600° are compared in Table IV.

TABLE IV

30-GROUP ELASTIC CROSS SECTIONS FOR ^{10}B AT 300 AND 600°K

Group	E_{MIN} (MeV)	E_{MAX} (MeV)	σ_{300} (barns)	σ_{600} (barns)
1	1.39 E-11	1.52 E-07	2.14100	2.24266
2	1.52 E-07	4.14 E-07	2.04519	2.05619
3	4.14 E-07	1.13 E-06	2.03793	2.04197
4	1.13 E-06	3.06 E-06	2.03501	2.03649
5	3.06 E-06	8.32 E-06	2.03344	2.03399
6	8.32 E-06	2.26 E-05	2.03199	2.03219
7	2.26 E-05	6.14 E-05	2.03050	2.03058
8	6.14 E-05	1.67 E-04	2.02752	2.02755
9	1.67 E-04	4.54 E-04	2.02518	2.02519
10	4.54 E-04	1.235 E-03	2.02040	2.02040
30	1.5 E+01	1.7 E+01	0.97914	0.97914

For further comparison, the MARK code[8] has been used to calculate group cross sections from the original ENDF/B tapes using the same boundaries and spectrum. MARK does not account for resonance or temperature effects, but in regions where these are negligible, agreement between MARK (ENDF/B format) and MRKACR (MCNP format) is excellent.

B. XSFICHE

The XSFICHE code provides interpreted microfiche listings of the data contained on MCNP cross-section tables. XSFICHE was executed for each table prepared during this work. Selected portions of the XSFICHE output for room-temperature ^{1}H are shown in Figs. 5-8. All abnormalities found in examining the microfiche have been investigated and corrected.

C. PLOTS

The XDATAP code has been used to generate many plots of the pointwise cross sections found on the new MCNP data tables. Several examples are shown in Figs. 9-11. In Fig. 9, the elastic scattering cross section of ^{1}H is plotted from 0-10 eV for 300° and 600°K. In Fig. 10, the radiative capture and fission cross sections of ^{238}U (room-temperature) are shown. Finally, Fig. 11 is a plot of the total, elastic, and capture cross sections of ^{135}Xe (room temperature). All plots generated have indicated satisfactory data and have been retained on microfiche.

D. TEST PROBLEMS

Various MCNP test problems were run with the new data sets. In particular, a simplified test problem obtained from L. Eisenhart of S. Levy Inc. was used to calculate criticality as a function of temperature. No problems were encountered and the results appeared reasonable.

At this point it was determined that the libraries should be turned over to the EPRI contractor. Clearly, with cross-section tables containing as many as 160,000 words of data, it is impossible to verify every number. However, the combined results of the integral data testing, differential plotting, interpreted microfiche listings, and MCNP test problems has convinced us that the likelihood of remaining major errors is exceedingly small.

IV. DATA AVAILABILITY

A. TRANSMISSION TO S. LEVY INC.

The data were transmitted to L. Eisenhart of S. Levy Inc. on July 20, 1987. The data were written onto a TK50 cartridge via a VAX computer at Los Alamos. Three files were written: the cross-section library, the associated directory, and a SPECS input file for the MAKXSF conversion code. The cross-section library was a 292,717-line BCD file containing 39 nuclear-data tables (18 continuous-energy neutron tables, 18 discrete-reaction neutron tables, 2 light-water $S(\alpha,\beta)$ tables, and 1 additional continuous-energy table for Hf). The data library was successfully read on a MICROVAX at S. Levy Inc.

B. GENERAL MCNP DATA BASE

As specified in the original contract, the data processed for EPRI will also be added to the general MCNP data base for all permissible users (because the data are based on ENDF/B-V, they cannot be transmitted to MCNP users outside the United States). This will be done in the near future at Los Alamos, at the National Magnetic Fusion Energy Center at Livermore, and for our external users through the Radiation Shielding Information Center at Oak Ridge.

C. USING THE DATA IN MCNP

The ZAIDs of the new data tables are defined in Table V. The ZAIDs one wishes to use are conveyed to MCNP via the Mn card(s). The associated cross-section directory file must be available to the code.

TABLE V

ZAID IDENTIFIERS OF HIGH-TEMPERATURE TABLES

Isotope	ZAID	Temperature (°K)	END	Temperature (MeV)
H-1	1001.53	300	4102	2.53 E-08
	1001.56	600	4062	5.06 E-08
B-10	5010.53	300	23737	2.53 E-08
	5010.56	600	23737	5.06 E-08
O-16	8016.53	300	38008	2.53 E-08
	8016.56	600	38050	5.06 E-08
	8016.59	900	38078	7.59 E-08
Zr	40000.53	300	58211	2.53 E-08
	40000.56	600	57569	5.06 E-08
Xe-135	54135.53	300	5570	2.53 E-08
	54135.56	600	5582	5.06 E-08
	54135.59	900	5618	7.59 E-08
U-235	92235.53	300	36429	2.53 E-08
	92235.56	600	36181	5.06 E-08
	92235.59	900	36069	7.59 E-08
U-238	92238.53	300	159552	2.53 E-08
	92238.56	600	160168	5.06 E-08
	92238.59	900	161032	7.59 E-08

One should ensure that the temperature of each cell in the MCNP problem is consistent with the temperature of the cross-section sets associated with the material of the cell. The temperatures (in MeV) are entered on the TMPn card(s).

V. CALCULATIONS

As mentioned in the introduction, several calculations have been performed with the high-temperature cross sections at Los Alamos. We have calculated k-effective and selected average cross sections. The input decks were obtained from L. Eisenhart and modified slightly. A sample input file is shown in Fig. 12.

Five detailed calculations were performed at Los Alamos. Each required ~75 minutes of CRAY X/MP-48 time. The five models calculated were: (1) 3.1% enrichment, hot zero power; (2) 3.1% enrichment, hot full power; (3) 1.6% enrichment, hot full power with Xenon; (4) 2.4% enrichment, hot full power with Xenon, and (5) 3.1% enrichment, hot full power with Xenon. The results for k-effective are summarized in Table VI. Notice that comparisons with CELL-2 results are excellent. Copies of all MCNP output files and listings of calculated average cross sections have been transmitted to L. Eisenhart.

TABLE VI

CALCULATED RESULTS FOR K-EFFECTIVE

Model	k-effective (MCNP)	k-effective (CELL-2)
3.1% enrichment, hot zero power	1.174 ± 0.003	1.177
3.1% enrichment, hot full power	1.165 ± 0.003	1.166
1.6% enrichment, hot full power, Xenon	0.921 ± 0.002	0.923
2.4% enrichment, hot full power, Xenon	1.065 ± 0.003	1.065
3.1% enrichment, hot full power, Xenon	1.148 ± 0.003	1.146

One final set of results indicates the sensitivity of thermal reactor criticality calculations to temperature. Hot zero power and hot full power calculations for the 3.1% enrichment case were repeated using room-temperature cross sections. The TMP1 card was unaltered for these runs. As a result, MCNP recognizes the "mismatch" between the temperatures of the cross-section sets and the temperatures of the cells and tries to account for it the best it can. The results are given in Table VII. From the calculated values of k-effective, one can see why the current work was necessary.

TABLE VII

MCNP CALCULATIONS WITH ROOM-TEMPERATURE CROSS SECTIONS

Model	k-effective	
	Room-Temp X-S	High-Temp X-S
3.1% enrichment, hot zero power	1.187 ± 0.003	1.174 ± 0.003
3.1% enrichment, hot full power	1.181 ± 0.003	1.165 ± 0.003

VI. SUMMARY

Neutron cross sections for several isotopes from ENDF/B-V have been Doppler-broadened to reactor temperatures and processed into a format appropriate for the MCNP Monte Carlo code. The data libraries have been thoroughly tested and verified. Cross-section tables have been transmitted to S. Levy Inc. and will be made available to the general MCNP user community. The high-temperature cross sections have been used in a variety of calculations at Los Alamos and S. Levy Inc. Monte Carlo results have been found to be in excellent agreement with results from the CELL-2 code.

REFERENCES

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2. Judith F. Briesmeister, Editor, "MCNP-A General Monte Carlo Code for Neutron and Photon Transport, Version 3A," Los Alamos National Laboratory manual LA-7396-M, Rev. 2 (September 1986).

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7. R. C. Little and R. E. Seamon, "Neutron-Induced Photon Production in MCNP," Proc. of the 6th Intl. Conf. on Radiation Shielding, Vol. I, 151 (May 1983).

8. R. E. Seamon, "The MARK and MRKACR Codes, "Los Alamos National Laboratory internal memorandum X-6:RES-87-182 to Distribution (March 26, 1987).

/samg

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X-6 Files (2)

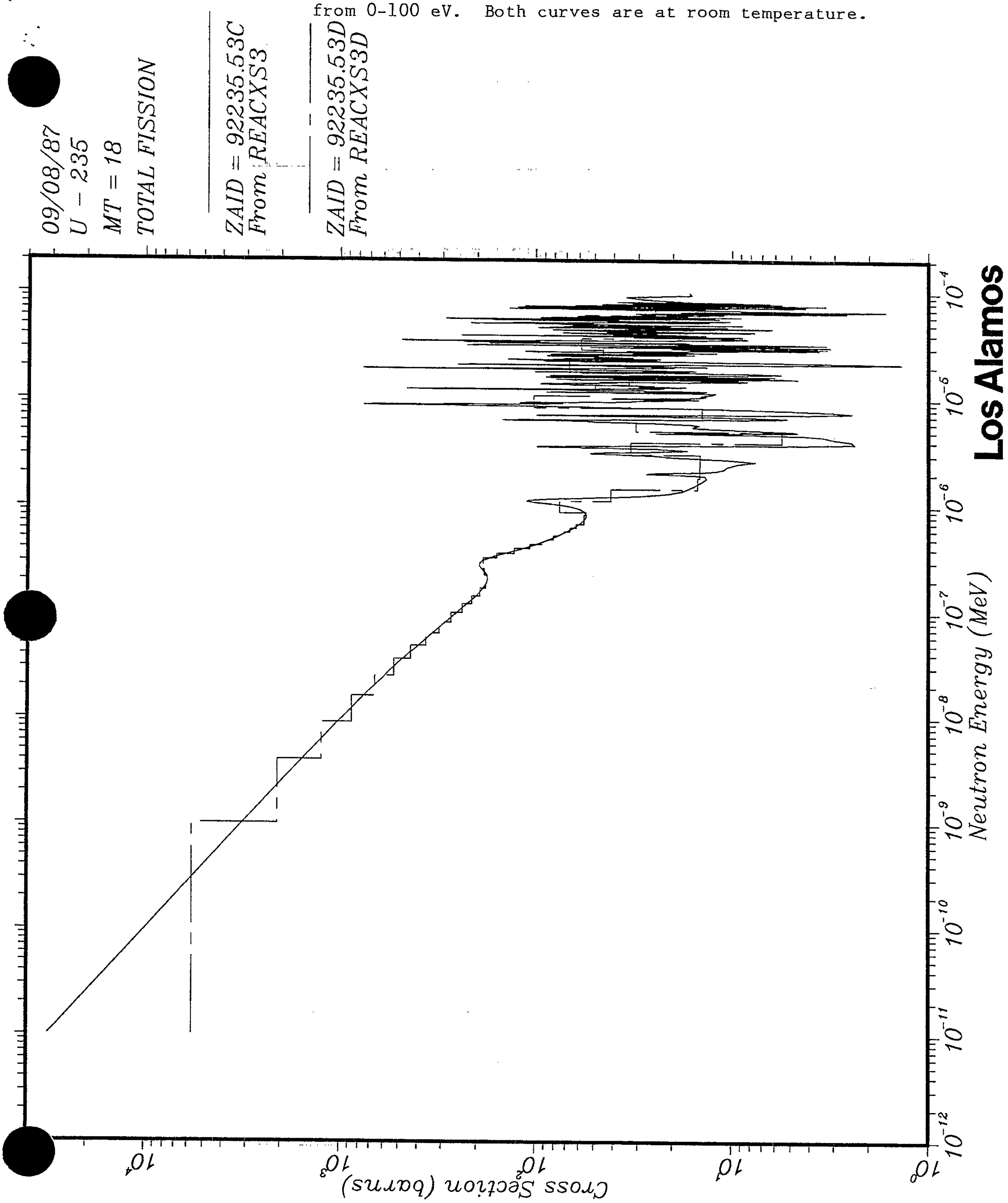
```
0
5
*RECONR*
-20 -21
*U235 MAT=1395 FROM TAPE 511* /
1395 /
.001 0 7 .001 /
0 /
*BROADR*
-21 -22
1395 3 0 0 0.
.001 /
300 600 900
0 /
*HEATR*
-20 -22 -23
1395 /
*STOP*
```

Fig. 1. Sample NJOY input file for creation of PENDF tape.

```
0
5
*GROUPR*
-20 -23 0 -24
1395 3 2 9 0 1 1 0
*U235* /
300
1.E+10
3 1 /
16 4 /
16 18 /
16 102 /
17 3 /
0 /
0 /
*ACER*
-20 -23 -24 25 26 /
0 1395 300 1 /
.001 /
-1 20000 1.E+10
*STOP*
```

Fig. 2. Sample NJOY input file for creation of ACE library.

Fig. 3. A comparison of the continuous-energy (solid) and discrete-reaction (broken) ^{235}U fission cross section from 0-100 eV. Both curves are at room temperature.



```
1001.53C 0.999170 XSNEW1 0 1 1 4041 0 0 2.5300E-08
1001.56C 0.999170 XSNEW1 0 1 1024 4001 0 0 5.0600E-08
5010.53C 9.926900 XSNEW1 0 1 2037 23676 0 0 2.5300E-08
5010.56C 9.926900 XSNEW1 0 1 7968 23676 0 0 5.0600E-08
8016.53C 15.858000 XSNEW1 0 1 13899 37947 0 0 2.5300E-08
8016.56C 15.858000 XSNEW1 0 1 23398 37989 0 0 5.0600E-08
8016.59C 15.858000 XSNEW1 0 1 32908 38017 0 0 7.5900E-08
40000.53C 90.436000 XSNEW1 0 1 42425 58170 0 0 2.5300E-08
40000.56C 90.436000 XSNEW1 0 1 56980 57528 0 0 5.0600E-08
54135.53C 133.748000 XSNEW1 0 1 71374 5529 0 0 2.5300E-08
54135.56C 133.748000 XSNEW1 0 1 72769 5541 0 0 5.0600E-08
54135.59C 133.748000 XSNEW1 0 1 74167 5577 0 0 7.5900E-08
92235.53C 233.025000 XSNEW1 0 1 75574 36368 0 0 2.5300E-08
92235.56C 233.025000 XSNEW1 0 1 84678 36120 0 0 5.0600E-08
92235.59C 233.025000 XSNEW1 0 1 93720 36008 0 0 7.5900E-08
92238.53C 236.006000 XSNEW1 0 1 102734 159491 0 0 2.5300E-08
92238.56C 236.006000 XSNEW1 0 1 142619 160107 0 0 5.0600E-08
92238.59C 236.006000 XSNEW1 0 1 182658 160971 0 0 7.5900E-08
1001.53D 0.999170 XSNEW1 0 1 222913 3210 0 0 2.5300E-08
1001.56D 0.999170 XSNEW1 0 1 223728 3210 0 0 5.0600E-08
5010.53D 9.926900 XSNEW1 0 1 224543 12813 0 0 2.5300E-08
5010.56D 9.926900 XSNEW1 0 1 227759 12813 0 0 5.0600E-08
8016.53D 15.858000 XSNEW1 0 1 230975 20455 0 0 2.5300E-08
8016.56D 15.858000 XSNEW1 0 1 236101 20455 0 0 5.0600E-08
8016.59D 15.858000 XSNEW1 0 1 241227 20455 0 0 7.5900E-08
40000.53D 90.436000 XSNEW1 0 1 246353 5855 0 0 2.5300E-08
40000.56D 90.436000 XSNEW1 0 1 247829 5855 0 0 5.0600E-08
54135.53D 133.748000 XSNEW1 0 1 249305 2869 0 0 2.5300E-08
54135.56D 133.748000 XSNEW1 0 1 250035 2869 0 0 5.0600E-08
54135.59D 133.748000 XSNEW1 0 1 250765 2869 0 0 7.5900E-08
92235.53D 233.025000 XSNEW1 0 1 251495 11789 0 0 2.5300E-08
92235.56D 233.025000 XSNEW1 0 1 254455 11789 0 0 5.0600E-08
92235.59D 233.025000 XSNEW1 0 1 257415 11789 0 0 7.5900E-08
92238.53D 236.006000 XSNEW1 0 1 260375 18818 0 0 2.5300E-08
92238.56D 236.006000 XSNEW1 0 1 265092 18818 0 0 5.0600E-08
92238.59D 236.006000 XSNEW1 0 1 269809 18818 0 0 7.5900E-08
LWTR.01T 0.000000 XSNEW1 0 1 274526 10193
LWTR.04T 0.000000 XSNEW1 0 1 277087 10193
72000.50C 176.954000 XSNEW1 0 1 279648 52231 0 0 2.5300E-08
```

Fig. 4. Cross-section directory file for new high-temperature data sets.

ZAID = 1001.53 NJOY NJOY (1301) 06/15/87

GAMMA PRODUCTION DATA =

ZAID	AWR	NTR	NES	NR	ESZ	MTR	TYR	LSIG	SIG
1001.53	0.999170	2	399	0	41	2037	2041	2043	2045

LAND	AND	LDLW	DLW	GPD	LQR		NU	FIS	END
2847	2848	3059	3059	3059	2039	100	0	0	4102

REACTION	MT	TYR	LSIG	LAND	LDLW	EMIN	EMAX	Q
ELASTIC	2			1		1.0000E-11	2.0000E+01	
(N,GMA)	102	0	1			1.0000E-11	2.0000E+01	2.2246E+00
DEUT PROD	204	0	402			1.0000E-11	2.0000E+01	0.0000E+00

Fig. 5. Portion of XSFICHE output for ^{1}H displaying counter and locator information as well as a summary of the available reactions.

ZAID = 1001.53 NJOY NJOY (1301) 06/15/87

I	ENERGY	TOTAL XS	ABSORPT. XS	ELASTIC XS	H AVE.	GAMMA PROD. XS
1	1.000000E-11	1.190515E+03	1.670446E+01	1.173810E+03	1.848501E-05	1.670446E+01
2	1.058199E-11	1.157333E+03	1.623876E+01	1.141095E+03	1.848486E-05	1.623876E+01
3	1.119194E-11	1.125363E+03	1.579005E+01	1.109573E+03	1.848471E-05	1.579005E+01
4	1.183091E-11	1.094561E+03	1.535772E+01	1.079203E+03	1.848455E-05	1.535772E+01
5	1.250000E-11	1.064872E+03	1.494104E+01	1.049931E+03	1.848439E-05	1.494104E+01
6	1.370255E-11	1.017088E+03	1.427041E+01	1.002818E+03	1.848417E-05	1.427041E+01
7	1.500000E-11	9.721217E+02	1.363927E+01	9.584825E+02	1.848385E-05	1.363927E+01
8	1.620987E-11	9.351540E+02	1.312039E+01	9.220336E+02	1.848355E-05	1.312039E+01
9	1.750000E-11	9.000382E+02	1.262754E+01	8.874107E+02	1.848332E-05	1.262754E+01
10	1.871524E-11	8.703400E+02	1.221072E+01	8.581293E+02	1.848308E-05	1.221072E+01
11	2.000000E-11	8.419353E+02	1.181200E+01	8.301233E+02	1.848276E-05	1.181200E+01
12	2.180790E-11	8.063001E+02	1.131179E+01	7.949883E+02	1.848232E-05	1.131179E+01
13	2.375000E-11	7.726494E+02	1.083941E+01	7.618100E+02	1.848185E-05	1.083941E+01
14	2.556775E-11	7.446942E+02	1.044699E+01	7.342473E+02	1.848141E-05	1.044699E+01
15	2.750000E-11	7.180729E+02	1.007328E+01	7.079997E+02	1.848096E-05	1.007328E+01
16	2.932508E-11	6.953850E+02	9.754780E+00	6.856302E+02	1.848053E-05	9.754780E+00
17	3.125000E-11	6.736441E+02	9.449564E+00	6.641945E+02	1.848006E-05	9.449564E+00
18	3.308074E-11	6.547538E+02	9.184366E+00	6.455694E+02	1.847964E-05	9.184366E+00
19	3.500000E-11	6.365641E+02	8.929024E+00	6.276351E+02	1.847924E-05	8.929024E+00
20	3.859841E-11	6.061935E+02	8.502667E+00	5.976909E+02	1.847847E-05	8.502667E+00
21	4.250000E-11	5.777277E+02	8.103028E+00	5.696246E+02	1.847764E-05	8.103028E+00
22	4.612309E-11	5.545981E+02	7.778261E+00	5.468198E+02	1.847679E-05	7.778261E+00
23	5.000000E-11	5.326892E+02	7.470619E+00	5.252186E+02	1.847588E-05	7.470619E+00
24	5.290995E-11	5.178528E+02	7.262291E+00	5.105905E+02	1.847523E-05	7.262291E+00
25	5.595969E-11	5.035634E+02	7.061626E+00	4.965018E+02	1.847451E-05	7.061626E+00
26	5.915455E-11	4.897961E+02	6.868280E+00	4.829278E+02	1.847376E-05	6.868280E+00
27	6.250000E-11	4.765273E+02	6.681928E+00	4.698454E+02	1.847296E-05	6.681928E+00
28	6.851273E-11	4.551718E+02	6.382029E+00	4.487897E+02	1.847167E-05	6.382029E+00
29	7.500000E-11	4.350769E+02	6.099767E+00	4.289771E+02	1.847013E-05	6.099767E+00
30	8.104936E-11	4.185575E+02	5.867709E+00	4.126898E+02	1.846870E-05	5.867709E+00
31	8.750000E-11	4.028667E+02	5.647274E+00	3.972194E+02	1.846717E-05	5.647274E+00
32	9.357618E-11	3.895975E+02	5.460841E+00	3.841367E+02	1.846572E-05	5.460841E+00
33	1.000000E-10	3.769070E+02	5.282529E+00	3.716244E+02	1.846421E-05	5.282529E+00
34	1.058199E-10	3.664228E+02	5.135203E+00	3.612876E+02	1.846283E-05	5.135203E+00
35	1.119194E-10	3.563256E+02	4.993321E+00	3.513323E+02	1.846144E-05	4.993321E+00
36	1.183091E-10	3.465978E+02	4.856603E+00	3.417412E+02	1.845993E-05	4.856603E+00
37	1.250000E-10	3.372226E+02	4.724830E+00	3.324978E+02	1.845835E-05	4.724830E+00
38	1.370255E-10	3.221344E+02	4.512734E+00	3.176217E+02	1.845551E-05	4.512734E+00
39	1.500000E-10	3.079381E+02	4.313148E+00	3.036250E+02	1.845247E-05	4.313148E+00
40	1.620987E-10	2.962688E+02	4.149059E+00	2.921197E+02	1.844962E-05	4.149059E+00
41	1.750000E-10	2.851856E+02	3.993190E+00	2.811924E+02	1.844660E-05	3.993190E+00
42	1.871524E-10	2.758136E+02	3.861358E+00	2.719522E+02	1.844372E-05	3.861358E+00
43	2.000000E-10	2.668510E+02	3.735267E+00	2.631158E+02	1.844068E-05	3.735267E+00
44	2.180790E-10	2.556091E+02	3.577063E+00	2.520320E+02	1.843634E-05	3.577063E+00
45	2.375000E-10	2.449954E+02	3.427686E+00	2.415677E+02	1.843180E-05	3.427686E+00
46	2.556775E-10	2.361801E+02	3.303589E+00	2.328765E+02	1.842755E-05	3.303589E+00
47	2.750000E-10	2.277872E+02	3.185413E+00	2.246017E+02	1.842305E-05	3.185413E+00
48	2.932508E-10	2.206358E+02	3.084696E+00	2.175511E+02	1.841881E-05	3.084696E+00
49	3.125000E-10	2.137845E+02	2.988182E+00	2.107963E+02	1.841435E-05	2.988182E+00
50	3.308074E-10	2.078327E+02	2.904320E+00	2.049284E+02	1.841011E-05	2.904320E+00
51	3.500000E-10	2.021030E+02	2.823555E+00	1.992795E+02	1.840557E-05	2.823555E+00
52	3.859841E-10	1.925393E+02	2.688705E+00	1.898506E+02	1.839713E-05	2.688705E+00
53	4.250000E-10	1.835790E+02	2.562320E+00	1.810167E+02	1.838811E-05	2.562320E+00
54	4.612309E-10	1.763017E+02	2.459633E+00	1.738420E+02	1.837981E-05	2.459633E+00
55	5.000000E-10	1.694113E+02	2.362362E+00	1.670490E+02	1.837096E-05	2.362362E+00

Fig. 6. Portion of XSFICHE output for 1[illegible]splaying major cross sections as a function of [illegible]gy.

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ANGULAR DISTRIBUTIONS FOR ELASTIC REACTION IN THE CENTER OF MASS SYSTEM

	ENERGY 1.000000E-11	ENERGY 1.000000E-01	ENERGY 1.000000E+00	ENERGY 1.000000E+01	ENERGY 1.600000E+01	ENERGY 2.000000E+01
1	-1.000000E+00	-1.000000E+00	-1.000000E+00	-1.000000E+00	-1.000000E+00	-1.000000E+00
2	-9.375000E-01	-9.375000E-01	-9.377632E-01	-9.394902E-01	-9.412268E-01	-9.425192E-01
3	-8.750000E-01	-8.750000E-01	-8.755101E-01	-8.787930E-01	-8.818948E-01	-8.841414E-01
4	-8.125000E-01	-8.125000E-01	-8.132408E-01	-8.179068E-01	-8.220888E-01	-8.250291E-01
5	-7.500000E-01	-7.500000E-01	-7.509550E-01	-7.568405E-01	-7.618605E-01	-7.652762E-01
6	-6.875000E-01	-6.875000E-01	-6.886517E-01	-6.956236E-01	-7.013056E-01	-7.050513E-01
7	-6.250000E-01	-6.250000E-01	-6.263311E-01	-6.342567E-01	-6.404285E-01	-6.443660E-01
8	-5.625000E-01	-5.625000E-01	-5.639932E-01	-5.727416E-01	-5.792299E-01	-5.832163E-01
9	-5.000000E-01	-5.000000E-01	-5.016389E-01	-5.110977E-01	-5.177800E-01	-5.217207E-01
10	-4.375000E-01	-4.375000E-01	-4.392683E-01	-4.493286E-01	-4.560987E-01	-4.599224E-01
11	-3.750000E-01	-3.750000E-01	-3.768813E-01	-3.874339E-01	-3.941836E-01	-3.978168E-01
12	-3.125000E-01	-3.125000E-01	-3.144771E-01	-3.254229E-01	-3.320668E-01	-3.354455E-01
13	-2.500000E-01	-2.500000E-01	-2.520553E-01	-2.632999E-01	-2.697710E-01	-2.728456E-01
14	-1.875000E-01	-1.875000E-01	-1.896161E-01	-2.010641E-01	-2.072946E-01	-2.100146E-01
15	-1.250000E-01	-1.250000E-01	-1.271596E-01	-1.387212E-01	-1.446502E-01	-1.469738E-01
16	-6.250000E-02	-6.250000E-02	-6.468586E-02	-7.627728E-02	-8.185888E-02	-8.376430E-02
17	0.000000E+00	0.000000E+00	-2.194989E-03	-1.373182E-02	-1.891967E-02	-2.038570E-02
18	6.250000E-02	6.250000E-02	6.031288E-02	4.891315E-02	4.415927E-02	4.314852E-02
19	1.250000E-01	1.250000E-01	1.228376E-01	1.116525E-01	1.073522E-01	1.067930E-01
20	1.875000E-01	1.875000E-01	1.853791E-01	1.744866E-01	1.706581E-01	1.705449E-01
21	2.500000E-01	2.500000E-01	2.479375E-01	2.374153E-01	2.340734E-01	2.343963E-01
22	3.125000E-01	3.125000E-01	3.105132E-01	3.004377E-01	2.975763E-01	2.983031E-01
23	3.750000E-01	3.750000E-01	3.731062E-01	3.635541E-01	3.611643E-01	3.622593E-01
24	4.375000E-01	4.375000E-01	4.357164E-01	4.267647E-01	4.248355E-01	4.262597E-01
25	5.000000E-01	5.000000E-01	4.983439E-01	4.900698E-01	4.885715E-01	4.902598E-01
26	5.625000E-01	5.625000E-01	5.609887E-01	5.534697E-01	5.523677E-01	5.542489E-01
27	6.250000E-01	6.250000E-01	6.236509E-01	6.169647E-01	6.162233E-01	6.182241E-01
28	6.875000E-01	6.875000E-01	6.863310E-01	6.805555E-01	6.801208E-01	6.821314E-01
29	7.500000E-01	7.500000E-01	7.490293E-01	7.442422E-01	7.440529E-01	7.459517E-01
30	8.125000E-01	8.125000E-01	8.117457E-01	8.080256E-01	8.080195E-01	8.096844E-01
31	8.750000E-01	8.750000E-01	8.744797E-01	8.719111E-01	8.720046E-01	8.732828E-01
32	9.375000E-01	9.375000E-01	9.372312E-01	9.359024E-01	9.359981E-01	9.367209E-01
33	1.000000E+00	1.000000E+00	1.000000E+00	1.000000E+00	1.000000E+00	1.000000E+00

Fig. 7. Portion of XSFICHE output for ^{1}H displaying elastic scattering angular distributions.

```
ZAID =    1001.53          NJOY                                  NJOY                    (1301) 06/15/87


 ENERGY DISTRIBUTION FOR SECONDARY PHOTONS FROM REACTION     (N,GMA) WITH  1 LAWS
                             MT=  102001


   LAW =   2      1ST OF  1 LAWS FOR REACTION     (N,GMA)
       PROBABILITY OF LAW
           NR =   0
           NE =   2
           E(I=1,NE) =    1.0000E-11  2.0000E+01
           P(I=1,NE) =    1.0000E+00  1.0000E+00

         DISCRETE PHOTON
       LP = 2  (PRIMARY PHOTON)
       EG = 2.22460
```

Fig. 8. Portion of XSFICHE output for ^{1}H displaying photon energy distribution from radiative capture.

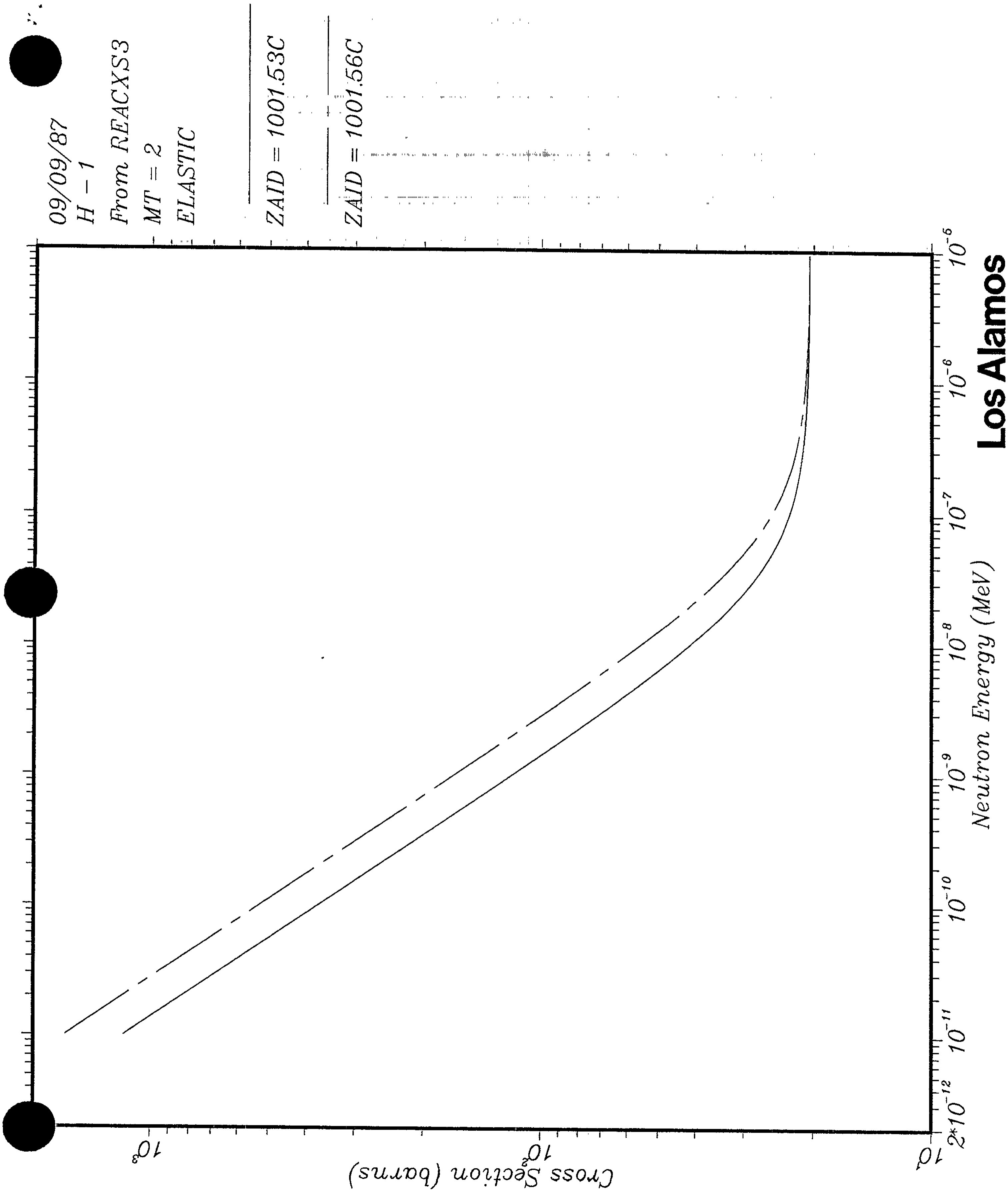


Fig. 9. The elastic scattering cross section of ^{1}H from 0-10 eV for 300° and 600°K.

Fig. 10. The radiative capture and fission cross sections of ^{238}U (room temperature).

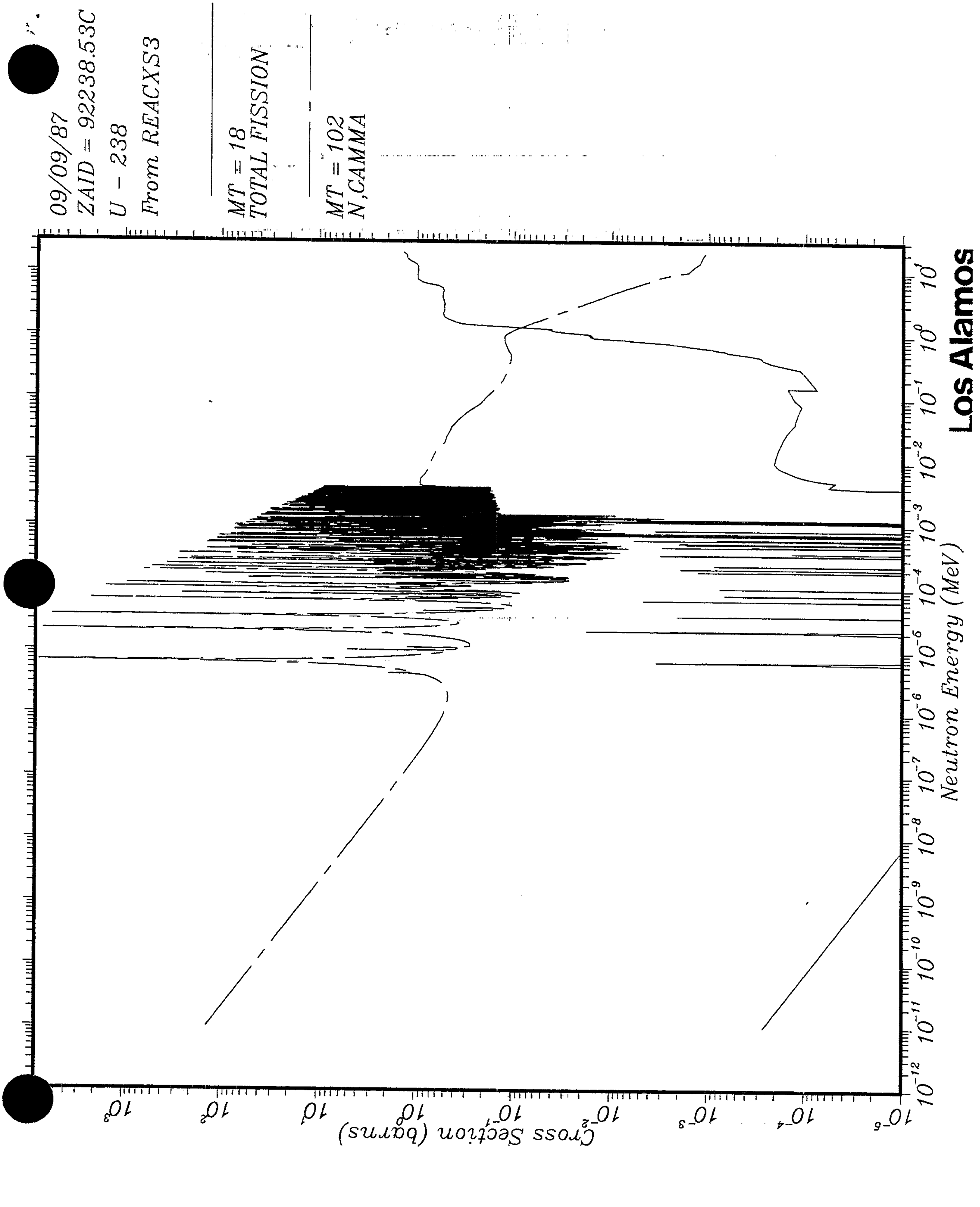
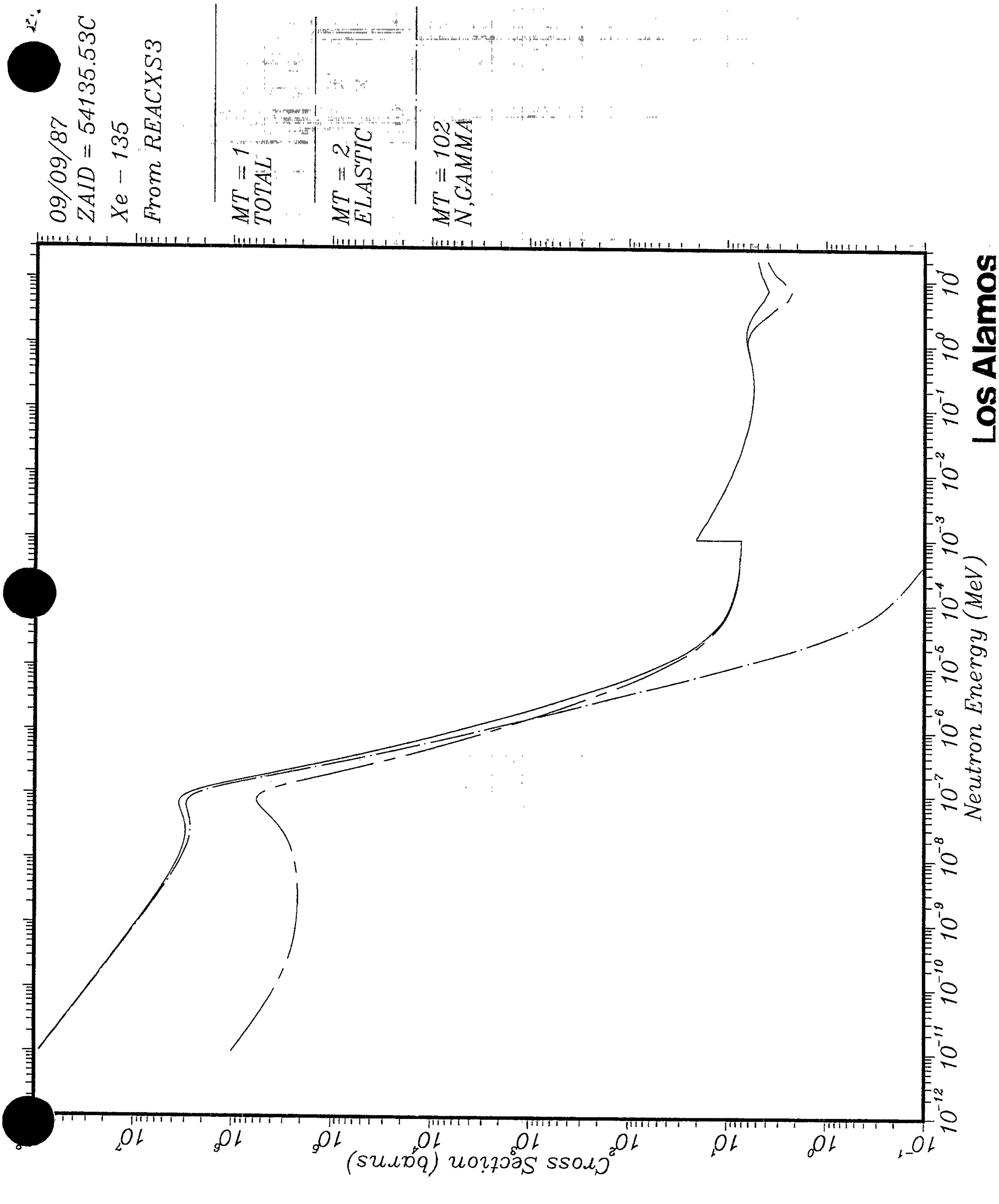


Fig. 11. The total, elastic, and capture cross sections of ^{135}Xe (room temperature).



```
MCNP3A-SINGLE ROD AT TMP=900+600/1400 PPM/3.10 % U-235 ROD+XENON
1       1  .0686526  -1 7 -8
2       2  .0389087  #1  -2 7 -8
3       3  .0663591  2 3 5 7 -4 -6 -8
4       0  #1 #2 #3

1       C/Z  0.0 0.0 0.39306
2       C/Z  0.0 0.0 0.45802
*3      PX   -0.63105
*4      PX   0.63105
*5      PY   -0.63105
*6      PY   0.63105
*7      PZ   -1000.0
*8      PZ   +1000.0

MODE  N
TMP   7.59E-8  5.06E-8 1R 0.0
NONU  1 2R 0
IMP:N    1 2R 0
AREA  2469.669 2877.825 2524.2  3R  2.537 1R
VOL    970.728 347.373  1867.692  1.E+10
KCODE 500   1.0 5 100  1250
KSRC  0.0 0.0 0.0
M1    92235.59 .0104614  92238.59 .322872  8016.59 .666667
       54135.59 .728305E-7
M2    40000.56 1.0
M3     1001.56 .666564  8016.56 .333282  5010.56 .000153909
MT3   LWTR.04
M51    92235.59 1.0
M52    92238.59 1.0
M60    54135.59 1.0
FQ0  U E
TOTNU
PRINT
F4:N      1
F44:N     1
E4    0.625E-6     5.531E-3   0.821  10.0
E44    0.625E-6     10.0
FM4      (1.0 51  (-2) (-2:-6) (-6) (-7) (-6 -7)) (1.0 60 (-2))
         (1.0 52 (-2) (-2:-6) (-6) (-7) (-6 -7))
      (1.0 1 (-2:-6) (-6) (-6 -7))
FM44      (1.0 51  (-2) (-2:-6) (-6) (-7) (-6 -7)) (1.0 60 (-2))
         (1.0 52 (-2) (-2:-6) (-6) (-7) (-6 -7))
      (1.0 1 (-2:-6) (-6) (-6 -7))
F64:N 2
FM64 1.0 2 -2
E64  .625E-06 5.531E-03 .821 10
F84:N 2
FM84 1.0 2 -2
E84  .625E-06 10
F104:N 3
FM104 1.0 3 -2
E104 .625E-06 5.531E-03 .821 10
F124:N 3
FM124 1.0 3 -2
E124 .625E-06 10
F184:N    1 2 3 T
F224:N    1 2 3 T
E184     0.625E-6     5.531E-3    0.821E+0   10.0
E224     0.625E-6     10.0
FM184      1.0
FM224      1.0
```

Fig. 12. Sample MCNP input file used for criticality calculation.

Charged–Particle Data Activities(R. C. Little and R. E. Seamon)

On August 17th we began a two–week period in which our activities were directed by T–Division consultant Leona Stewart. She came with the stated goal of setting priorities on the list of charged–particle reactions. At her instigation, a meeting was held on August 19 "to discuss the needs and priorities for evaluated libraries for charged–particles incident." The quotation is from the minutes of that meeting which were published as Ref. 1. At that meeting, Thurman Talley, T–2, presented an 18 page list entitled "Plasma Data Priority" in which over 430 (four hundred and thirty) reactions between particles n, p, d, t, ^{3}He, α, ^{6}He, ^{6}Li, ^{7}Li, ^{8}Li, ^{9}Li, ^{7}Be, ^{9}Be, ^{11}Be, ^{8}B, ^{10}B, and ^{11}B were suggested as being of possible concern in weapons design calculations. "It was generally agreed that we should focus on data for ^{6}Li at this time and confine our efforts to the reaction channels....... " (Quote from Ref. 1). There was much concern expressed about the "completeness and reliability of the data currently in the ECPL library " (Quote from Ref. 1). The ECPL library referred to is the 1986 version of the Livermore Evaluated Charged Particle Library; details concerning structure of the 1984 version of ECPL as we had it available in Los Alamos were given in Ref. 2. Most of the multigroup data to be found on CPFILE, the multigroup X–Division Charged Particle Library (Ref. 3) have been processed from the 1986 version of ECPL. It became quite apparent that the attacks on the integrity of ECPL had to be answered or else the integrity of the various editions of CPFILE would be under question.

Another meeting of the group was scheduled for August 26, the minutes for which appeared as Ref. 4. We were charged with the preparation of the following items "for perusal at (that) meeting." (Quote from Ref. 1):

1. A list of the reactions available on the 1986 edition of ECPL. That list appears in this report as Table I.
2. A summary of all charged–particle reactions on ^{6}Li targets suggested by Gula, Stewart, and Talley. That list of 46 reactions is given in Table II along with the Q values which we calculated and checked where possible against Howerton's list in Ref. 5. Cross sections for the starred reactions in Table II are available on the 1986 version of ECPL. Of the 46 reactions listed, there are only 13 starred reactions.
3. A summary of all charged–particle reactions on ^{7}Li targets suggested by Gula, Stewart, and Talley. In a manner similar to that for the ^{6}Li reactions, that list is given in Table III along with the Q values. Of the 42 reactions listed, cross sections for 13 are available on the 1986 version of ECPL.
4. Plots of the 20 available charged–particle reaction cross sections on ^{6}Li from the 1986 version of ECPL were prepared.
5. Plots of the 18 available charged–particle reaction cross sections on ^{7}Li from the 1986 version of ECPL were prepared.
6. Over 113 experimental values were read from figures found in the literature and plotted onto figures with the ECPL curves for the following six reactions:

$$^6\mathrm{Li}(p,{}^3\mathrm{He})\alpha$$

$$^6\mathrm{Li}(d,n)^7\mathrm{Be} + \gamma$$

$$^6\mathrm{Li}(d,n^3\mathrm{He})\alpha$$

$$^6\mathrm{Li}(d,p)^7\mathrm{Li} + \gamma$$

$$^6\mathrm{Li}(d,pt)\alpha$$

$$^6\mathrm{Li}(d,\alpha)\alpha$$

That work in defense of the cross sections on ECPL has been greatly extended during the remainder of this report period. We have looked at all papers which Lee called to our attention plus many more we found ourselves in the literature. The experimental values have been read from figures therein and are now available in computerized form for use in computerized comparisons with the ECPL pointwise evaluated data. A brief summary of the contents of that file is given in Table IV.

7. Experimental data from Don Barr have been compared with the ECPL curves for the following seven reactions in which ^{7}Be is one of the final products:

$$^{6}\mathrm{Li(d,n)}^{7}\mathrm{Be} + \gamma$$

$$^{6}\mathrm{Li(t,2n)}^{7}\mathrm{Be} + \gamma$$

$$^{6}\mathrm{Li(}^{3}\mathrm{He,d)}^{7}\mathrm{Be} + \gamma$$

$$^{7}\mathrm{Li(p,n)}^{7}\mathrm{Be} + \gamma$$

$$^{7}\mathrm{Li(d,2n)}^{7}\mathrm{Be} + \gamma$$

$$^{7}\mathrm{Li(t,3n)}^{7}\mathrm{Be} + \gamma$$

$$^{7}\mathrm{Li(}^{3}\mathrm{He,t)}^{7}\mathrm{Be} + \gamma$$

It is quite clear from those comparisons that Howerton was influenced by the Barr measurements.
8. Statements concerning the characteristics of secondary distributions on ECPL for reactions with ^{6}Li and ^{7}Li.

It was quite clear even to Lee before the second meeting (August 26th) that the efforts under Items 6 and 7 above would substantially refute the criticisms of the ECPL cross section evaluations. She turned then her attention to the energy and angular distributions of the residual nucleons and nuclei as found on ECPL. For example, in Ref. 6 she correctly pointed out that something is wrong with two photon energy distributions. We have looked at that problem and understand more or less what happened in the preparation of the ECPL numbers. A memo on that topic is yet to be written.

These matters as discussed so far were presented at the ^{7}Be Working Group meeting on October 5th. What was NOT mentioned at that meeting, an oversight on Seamon's part, was the fact that Little has processed into multigroup format using the Livermore code CLYDE (Ref. 7) most of the reactions listed in Table I for targets p, d, t, ^{3}He, α, ^{6}Li, and ^{7}Li. It is understood that these data are not yet available on CPFILE, but the monumental multigrouping task has been essentially completed. Said in another way, just suppose for a moment that we had tables like Tables II and III available for all the targets just mentioned. Then, multigroup cross sections would be processed for all the "starred" reactions. It may very well be that this "integral" approach is the best way to "defend" ECPL; soon the multigroup numbers will be available on CPFILE; they can be used and we'll see how the calculated quantities compare with results from some of the weapons shots.

There is an incorrect notion in the minds of some T-Division management that the devastation of the two work weeks August 17–28 really "got us on the ball." Those who have perused the Activity Reports from Group X-6 will realize that charged-particle concerns have manifest themselves quite literally for years. After all, many of the changes in MCNP introduced for Version 3B have been made with a foresight that MCNP will become an N-particle code (see Hendricks' Ref. 7). But never mind visions. What about all the work that is made manifest in the early versions of CPFILE, the format for which was initially described in 1985 (Ref. 8) and the first version of which was available at that time. It might be well for our critics to be reminded of Little's report on the Group X-6 activities in the areas of charged-particle reactions, transport, and data; they could read it in Ref. 9.

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Table I

Reactions Considered on the 1986 Version of ECPL

$t + p \rightarrow n + {}^3He$

$d + d \rightarrow n + {}^3He$
$t + d \rightarrow n + \alpha$
$\alpha + d \rightarrow n + p + \alpha$
$\alpha + d \rightarrow p + n + \alpha$
$t + d \rightarrow n + \alpha + \gamma$
$d + d \rightarrow p + t$
${}^3He + d \rightarrow p + \alpha$

$p + t \rightarrow n + {}^3He$
$d + t \rightarrow n + \alpha$
$t + t \rightarrow 2n + \alpha$
$d + t \rightarrow n + \alpha + \gamma$
$p + t \rightarrow \gamma + \alpha$

$t + {}^3He \rightarrow n + p + \alpha$
$t + {}^3He \rightarrow p + n + \alpha$
$d + {}^3He \rightarrow p + \alpha$
$t + {}^3He \rightarrow d + \alpha$

$p + {}^7Li \rightarrow n + {}^7Be + \gamma$
$t + {}^7Li \rightarrow n + {}^9Be$
$d + {}^7Li \rightarrow 2n + {}^7Be + \gamma$
$t + {}^7Li \rightarrow 3n + {}^7Be + \gamma$
$d + {}^7Li \rightarrow n + 2\alpha$
$t + {}^7Li \rightarrow 2n + 2\alpha$
${}^3He + {}^7Li \rightarrow n + p + 2\alpha$
${}^3He + {}^7Li \rightarrow p + {}^9Be$
${}^3He + {}^7Li \rightarrow t + {}^7Be + \gamma$
$p + {}^7Li \rightarrow 2\alpha$
${}^3He + {}^7Li \rightarrow \alpha + {}^6Li$
${}^3He + {}^7Li \rightarrow \alpha + {}^6Li + \gamma$ (3.562 MeV)
${}^3He + {}^7Li \rightarrow d + 2\alpha$

$d + {}^6Li \rightarrow n + {}^7Be + \gamma$
$t + {}^6Li \rightarrow 2n + {}^7Be + \gamma$
$d + {}^6Li \rightarrow n + {}^3He + \alpha$
$t + {}^6Li \rightarrow n + 2\alpha$
$d + {}^6Li \rightarrow p + t + \alpha$
$d + {}^6Li \rightarrow p + {}^7Li + \gamma$
$\alpha + {}^6Li \rightarrow p + {}^9Be$
$t + {}^6Li \rightarrow d + {}^7Li$
$t + {}^6Li \rightarrow d + {}^7Li + \gamma$ (0.994 MeV)
${}^3He + {}^6Li \rightarrow d + {}^7Be + \gamma$
$p + {}^6Li \rightarrow {}^3He + \alpha$
$d + {}^6Li \rightarrow 2\alpha$
$\alpha + {}^6Li \rightarrow d + 2\alpha$
${}^3He + {}^6Li \rightarrow p + 2\alpha$

$t + {}^7Be \rightarrow d + 2\alpha$
$d + {}^7Be \rightarrow p + 2\alpha$

Also:
(1) Large–angle Coulomb and Nuclear Elastic plus Interference are provided for all combinations of p, d, t, ${}^3He$, α as projectile and target.
(2) Large–angle Coulomb is provided for p, d, t, ${}^3He$, α on targets of ${}^6Li$, ${}^7Li$, and ${}^7Be$.
(3) Some data are also provided for the following targets: ${}^9Be$, ${}^{10}B$, ${}^{11}B$, ${}^{12}C$, ${}^{14}N$, ${}^{16}O$, and ${}^{89}Y$

Table II

Charged–Particle Reactions on ^{6}Li Targets

	Reaction	Q(MeV)		Reaction	Q(MeV)
	^{6}Li(p,p)^{6}Li elastic	0.0		^{6}Li(t,2n)^{3}He α	–4.462
	^{6}Li(p,γ)^{7}Be	5.606		^{6}Li(t,p)^{8}Li	0.802
	^{6}Li(p,n2p)α	–3.698	⋆	^{6}Li(t,d)^{7}Li	0.994
	^{6}Li(p,pd)α	–1.474		^{6}Li(t,dt)α	–1.4736
	^{6}Li(p,d)^{5}Li	–3.404		^{6}Li(t,^{3}He)^{6}He	–3.491
	$\hookrightarrow$p + α	–1.474		^{6}Li(t,α)^{5}He	15.248
⋆	^{6}Li(p,^{3}He)α	4.020		$\hookrightarrow$n + α	16.116
	^{6}Li(d,d)^{6}Li elastic	0.0		^{6}Li(^{3}He,^{3}He)^{6}Li elastic	0.0
⋆	^{6}Li(d,n)^{7}Be + γ	3.3817		^{6}Li(^{3}He,γ)^{9}B	16.602
	^{6}Li(d,pn)^{6}Li	–2.224		^{6}Li(^{3}He,n)^{8}B	–1.974
	^{6}Li(d,pnd)α	–3.698	⋆	^{6}Li(^{3}He,p)2α	16.880
	^{6}Li(d,2n)^{6}Be	–7.289		^{6}Li(^{3}He,p)^{8}Be	16.787
	^{6}Li(d,2n2p)α	–5.922		$\hookrightarrow$2α	16.880
⋆	^{6}Li(d,n^{3}He)α	1.796		^{6}Li(^{3}He,2p)^{7}Li	–0.469
⋆	^{6}Li(d,p)^{7}Li + γ	5.026		^{6}Li(^{3}He,pn)^{7}Be	–2.112
⋆	^{6}Li(d,pt)α	2.560	⋆	^{6}Li(^{3}He,d)^{7}Be + γ	0.11206
	^{6}Li(d,2d)α	–1.4736		^{6}Li(^{3}He,t)^{6}Be	–4.301
	^{6}Li(d,^{3}He)^{5}He	0.928		$\hookrightarrow$2p + α	–2.934
	$\hookrightarrow$n + α	1.796		^{6}Li(^{3}He,α)^{5}Li	14.950
⋆	^{6}Li(d,α)α	22.375		^{6}Li(α,α)^{6}Li elastic	0.0
	^{6}Li(t,t)^{6}Li elastic	0.0		^{6}Li(α,γ)^{10}B	4.462
	^{6}Li(t,γ)^{9}Be	17.689		^{6}Li(α,n)^{9}B	–3.976
⋆	^{6}Li(t,n)2α	16.116		^{6}Li(α,np)2α	–3.698
	^{6}Li(t,n)^{8}Be	16.024	⋆	^{6}Li(α,p)^{9}Be	–2.125
	$\hookrightarrow$2α	16.116	⋆	^{6}Li(α,d)2α	–1.474
⋆	^{6}Li(t,2n)^{7}Be + γ	–2.8762		^{6}Li(α,t)^{7}Be	–14.208

Table III

Charged–Particle Reactions on ^{7}Li Targets

	Reaction	Q(MeV)
	^{7}Li(p,p)^{7}Li elastic	0.0
	^{7}Li(p,γ)^{8}Be	17.256
	$\hookrightarrow 2\alpha$	17.348
*	^{7}Li(p,n)^{7}Be + γ	-1.64379
	^{7}Li(p,d)^{6}Li	-5.025
	^{7}Li(p,t)^{5}Li	-4.396
	^{7}Li(p,^{3}He)^{5}He	-4.098
*	^{7}Li(p,α)α	17.348
	^{7}Li(d,d)^{7}Li elastic	0.0
*	^{7}Li(d,n)2α	15.124
*	^{7}Li(d,2n)^{7}Be + γ	-3.8682
	^{7}Li(d,p)^{8}Li	-0.191
	^{7}Li(d,t)^{6}Li	-0.994
	^{7}Li(d,dt)α	-2.466
	^{7}Li(d,^{3}He)^{6}He	-4.483
	^{7}Li(d,α)^{5}He	14.256
	$\hookrightarrow$ n + α	15.124
	^{7}Li(t,t)^{7}Li elastic	0.0
	^{7}Li(t,γ)^{10}Be	17.251
*	^{7}Li(t,n)^{9}Be	10.439
*	^{7}Li(t,2n)2α	8.866
*	^{7}Li(t,3n)^{7}Be + γ	-10.1260
	^{7}Li(t,p)^{9}Li	-2.385
	^{7}Li(t,d)^{8}Li	-4.224
	^{7}Li(t,α)^{6}He	9.838
	$\hookrightarrow$ 2n + α	8.866

	Reaction	Q(MeV)
	^{7}Li(^{3}He,^{3}He)^{7}Li elastic	0.0
	^{7}Li(^{3}He,γ)^{10}B	17.790
	^{7}Li(^{3}He,n)^{9}B	9.352
	^{7}Li(^{3}He,2n)^{8}B	-9.225
*	^{7}Li(^{3}He,p)^{9}Be	11.203
*	^{7}Li(^{3}He,pn)2α	9.630
*	^{7}Li(^{3}He,d)2α	11.854
	^{7}Li(^{3}He,d)^{8}Be	11.762
	$\hookrightarrow 2\alpha$	11.854
*	^{7}Li(^{3}He,t)^{7}Be + γ	-0.880
*	^{7}Li(^{3}He,α)^{6}Li	13.328
*	^{7}Li(^{3}He,α)^{6}Li*(3.562 MeV) + γ	
	^{7}Li(α,α)^{7}Li elastic	0.0
	^{7}Li(α,n)^{10}B	-2.788
	^{7}Li(α,2n)^{9}B	-11.225
	^{7}Li(α,p)^{10}Be	-2.563
	^{7}Li(α,d)^{9}Be	-7.150
	^{7}Li(α,t)2α	-2.466
	^{7}Li(α,^{5}He)^{6}Li	-8.118
	^{7}Li(α,^{6}He)^{5}Li	-11.907
	$\hookrightarrow$ p + α	-9.977

Table IV

Status Report

Computerized File of Experimental Cross Section Values

Reaction	Number of σ Measurements	
$^6Li(p,^3He)\alpha$	70	
$^6Li(^3He,p)$	96	proton production
$^6Li(d,n)^7Be$	102	
$^6Li(d,\alpha)\alpha$	323	
$^6Li(d,p)^7Li$	79	
$^6Li(d,n^3He)\alpha$	5	
$^6Li(d,pt)\alpha$	6	
$^6Li(t,n)2\alpha$	8	
$^6Li(t,p)^8Li$	46	
$^6Li(\alpha,p)^9Be$	77	
$^6Li(p,p)^6Li$	406	differential measurements
$^7Li(t,2n)2\alpha$	10	

A New Subroutine for DITTO(R. C. Little)

In Ref. 1 I described an expansion to the format of our random–access multigroup libraries like MENDF5 and RMOXSCT which enables us to incorporate information about the reaction products for each reaction. The constraint applied is that each reaction product must be either a neutron or an isotope for which cross–section data exist on the library. The assumptions made when data for a true reaction product do not exist on the library are detailed in Ref. 1, but in general I have tried to conserve mass as best as possible in such cases.

During this report period I have written a subroutine to replace Subroutine GETNR in DITTO; the new subroutine, which is approximately 150 lines long, is described in Ref. 2. It helps DITTO set up the reaction chains for the depletion calculations. There are five calling variables:

1. ISO – isotope ZAID (1000*Z+A) for which reaction–product data are desired.
2. NRFLAG – user option that selects which suite of reactions to follow.
   NRFLAG=1 – follow all available reactions.
   NRFLAG=2 – follow only those reactions available on the RMOXSCT library.
   NRFLAG=3 – follow the special GOK reactions only.
3. NEWFP – user option that selects which fission product cross sections to use.
   NEWFP=0 – use the old Los Alamos fission product pair (FPA):ISO=50999.
   NEWFP=1 – use the new Los Alamos fission products:
   ISO=45117 for fissionable isotopes with $Z \leq 93$;
   ISO=46119 for fissionable isotopes with $Z \geq 94$.
   NEWFP=2 – use the new Livermore fission product: ISO=50120.
4. NPFLAG – user option that further limits the reactions to be followed.
   NPFLAG=± 2 – don't follow and (n,p) or (n,α) reactions (for $6<Z<90$).
   NPFLAG=± 3 – don't follow any reactions (for $6<Z<90$).
5. JNX – unit number for the cross–section library.

In the coding for the current version of DITTO, an attempt is made to conserve Z for the cases when the true reaction products do not exist; as discussed above, I am now trying to conserve A. It is for this reason that numerical results obtained with the new Subroutiune GETNR2 may not agree with calculations obtained using the original Subroutine GETNR. Despite the different assumptions, I don't believe that there are different reaction products for any important reactions, and the calculated quantities of interest should vary only slightly.

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